Nuclear Fuel Cycle (NFC) Systems Studies Activities at Los Alamos

Advanced Accelerator Applicatio

Chuck Bathke

Wiley Davidson

Bob Krakowski

Chris Lovejoy

Shelly Spearing

Holly Trellue

AAA Third Quarterly Technical Review

Washington, DC

July 9-10, 2002

Los Alamos National Laboratory

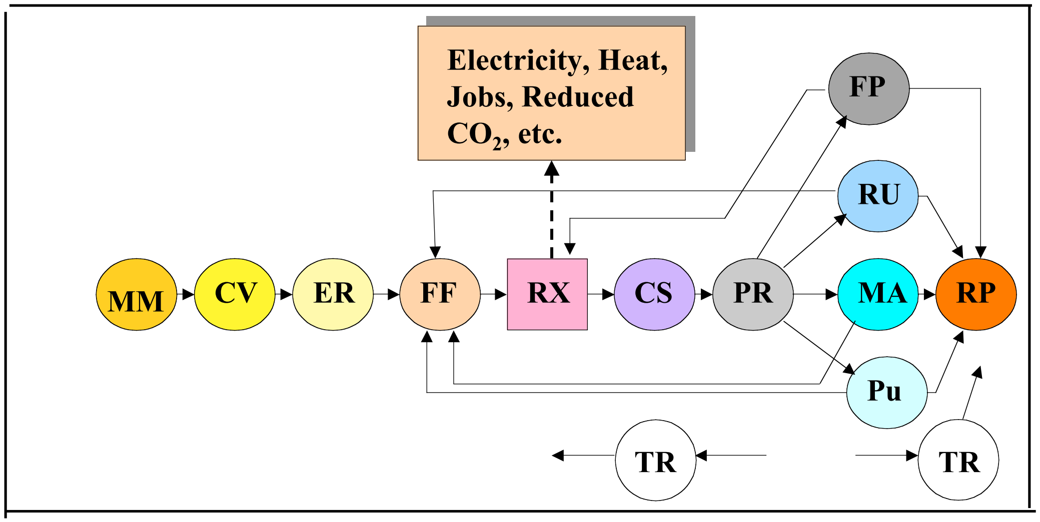
Group D-3, MS F607

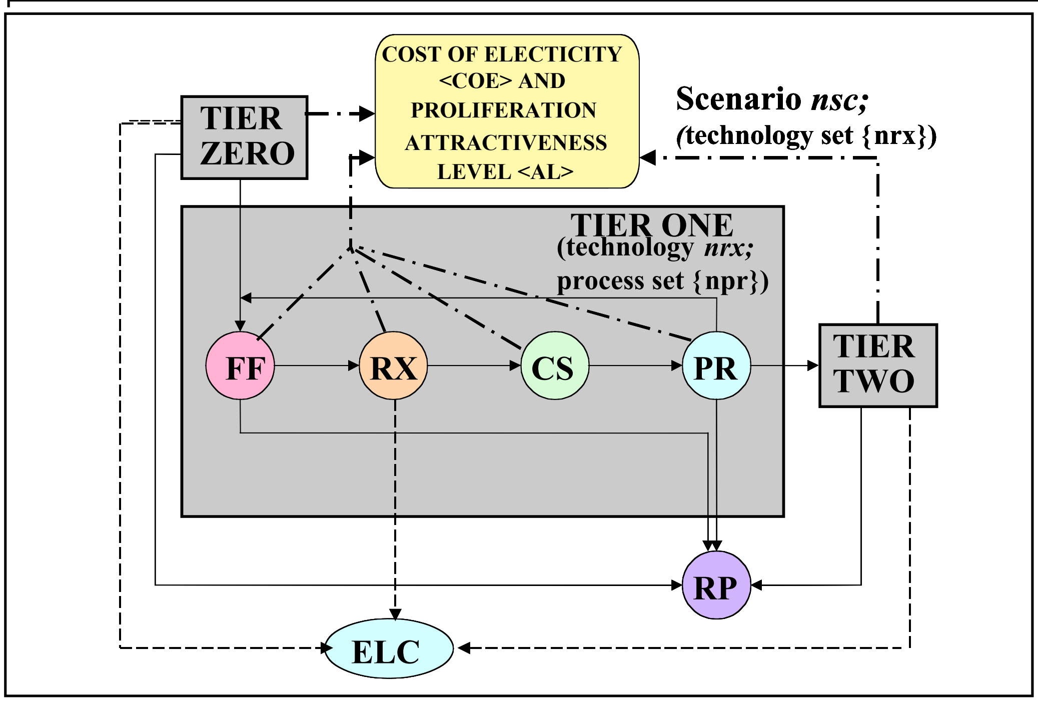
Los Alamos, New Mexico, 87545, USA

AAA Nuclear Fuel Cycle (NFC) Systems Analyses Effort at Los Alamos: Contents

Advanced Accelerator Applicatio

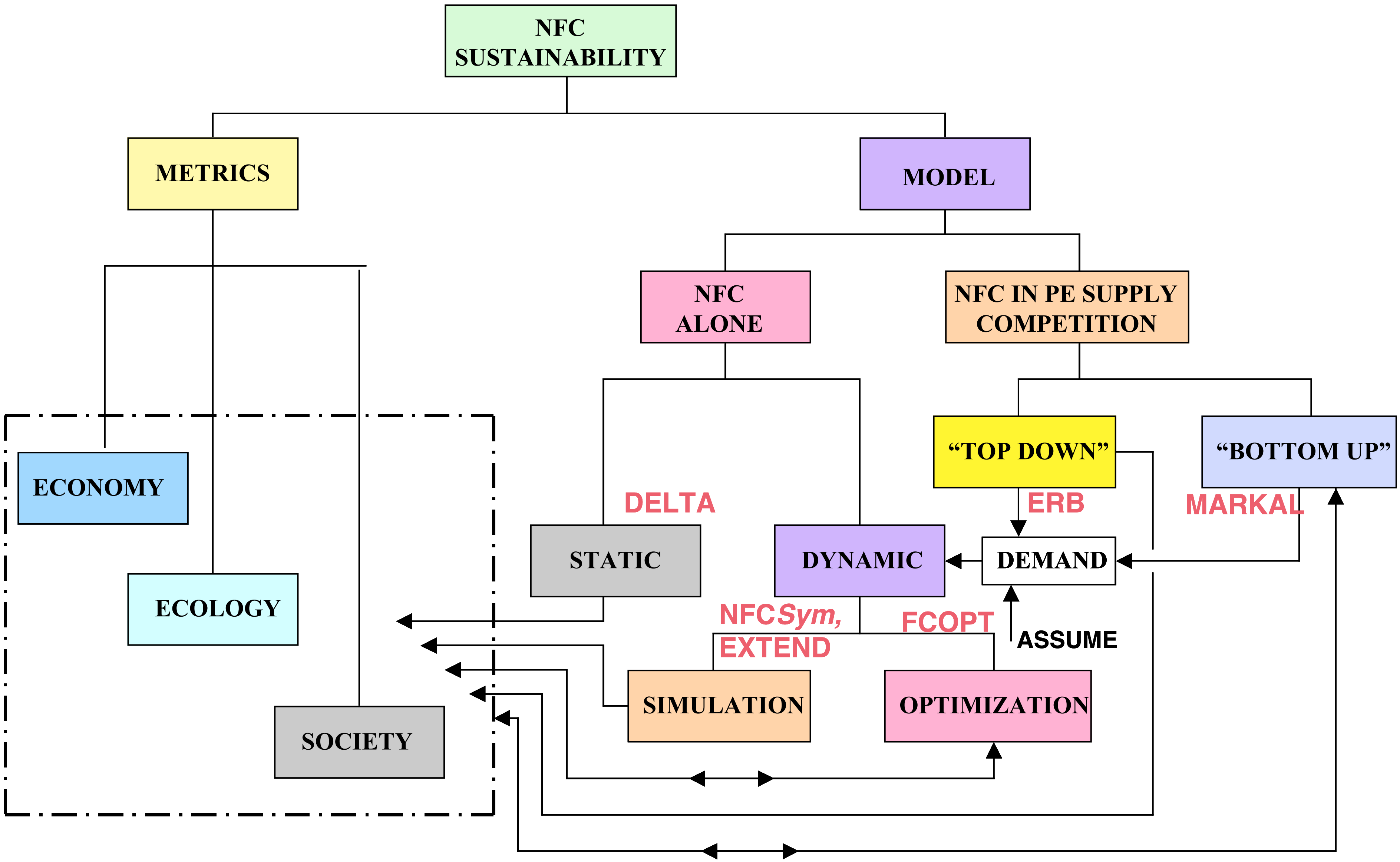
General Approach to Nuclear Fuel Cycle Analyses Used in AAA Project





- Scope scenario options/impacts using equilibrium (steady-state), "top-level" (aggregated processes) NFC Model;
- Evaluate scenarios based on a range of performance indicators or metrics (*e.g.*, cost, waste mitigation, proliferation risk, resource utilization);
- Build scenarios based on coupled technologies presented in a *multi-tiered* configuration;
- Based on equilibrium analyses, perform *dynamic simulations* and *optimizations* on limited number of scenarios.

NFC Modeling Relationships, Scope, and Options



Main Accomplishments for Third Quarter FY02

- **Document equilibrium NFC (DELTA) model and results used to support AAARC[a];**
- **Initiate development of NFC dynamic *simulation model* (NFCSym, supported by parallel development of an EXTEND™ scoping model;**
- **Initiate development of NFC *optimization model* (FCOPT) to support (provide directions to) NFCSym;**
- **Database and neutronics support for both NFCSym and FCOPT;**
- **Initiate dynamic NFC modeling benchmark collaboration between CEA (COSI) and Los Alamos (NFCSym);**
- **Begin assessment of impact of a range of front-end ("thin", "tier-less") processing scenarios on repository volume and heat-load requirements.**

---

[a] R. A. Krakowski and C. G. Bathke, "Method for Quantitative Assessment of Cost and Proliferation Risks Associated with the Civilian Nuclear Fuel Cycle as Applied to the Advanced Accelerator Applications (AAA) Program," Los Alamos National Laboratory document LA-UR-02-2369 (April 26, 2002)

Plans for Rest of FY02

- Complete preliminary development of and report on NFC *simulation model* (NFCSym, supported by simplified EXTEND™ model), including:
  - begin introduction of rudimentary neutronics into NFCSym;
  - complete package for tallying inventories at nuclear sites;
  - complete economics/costing package.
- Define NFC scenario for COSI(CEA) – NFCSym benchmark; prepare for preliminary comparison (database, neutronics, *etc*.)
- Complete preliminary development of and report on NFC *optimization model* (FCOPT), and integrate with NFCSym *simulation model*;
- Complete examination of and report YM volume and heat-load impacts base on series of front-end ("thin", "tier-less") scenarios.

Approximate Time Lines for Key AAA Systems Studies Technical Activities at Los Alamos

Modeling Approach =>	Simulation										Optimzation				
Technical Activity	**NFCSim**					**EXTEND™**					**FCOPT**				
NFC Mass/Power Flows															
o full NFC for Tier-0															
o full NFC for Tier-1															
o full NFC for Tier-2															
Mass Flow Fidelity															
o bulk lots (e.g., FF, SNF, etc.)															
o MA, Pu, FP, RU, etc.															
o isotopics															
Core Physics (Neutronics)															
o extrinsic (LANL, ANL)															
o intrinsic (point model)															
Metrics															
o costing															
o proliferation															
o waste															
Benchmarks															
o intrinsic (NFCSim, Extend™, FCOPT)															
o extrinsic [ANL, CEA(?)]					?					?					?

APR02 — **OCT02, APR02** — **OCT02, APR02** — **OCT02**

Activities Planned for FY03

➢ **Focus primarily on CEA-LANL/ANL dynamic NFC model benchmarking (COSI-NFCSym):**

- bring NFCSym neutronics to comparable level used in COSI;

- align processing and neutronics databases;

- finalize NFC scenarios to be compared in terms of tier-structure and country (France, USA, 'Utopia'?);

- settle on short- and long-term repository impacts to be investigated.

➢ **Continue NFCSym *simulation model* development, in parallel with *optimization model* (FCOPT);**

➢ **Initiate development of NFC optimization model in a broader (US) energy context (MARKAL).**

Background/Amplifying Material

DELTA Model[a] : A Steady-State (Equilibrium) Nuclear Fuel Cycle (NFC) Model

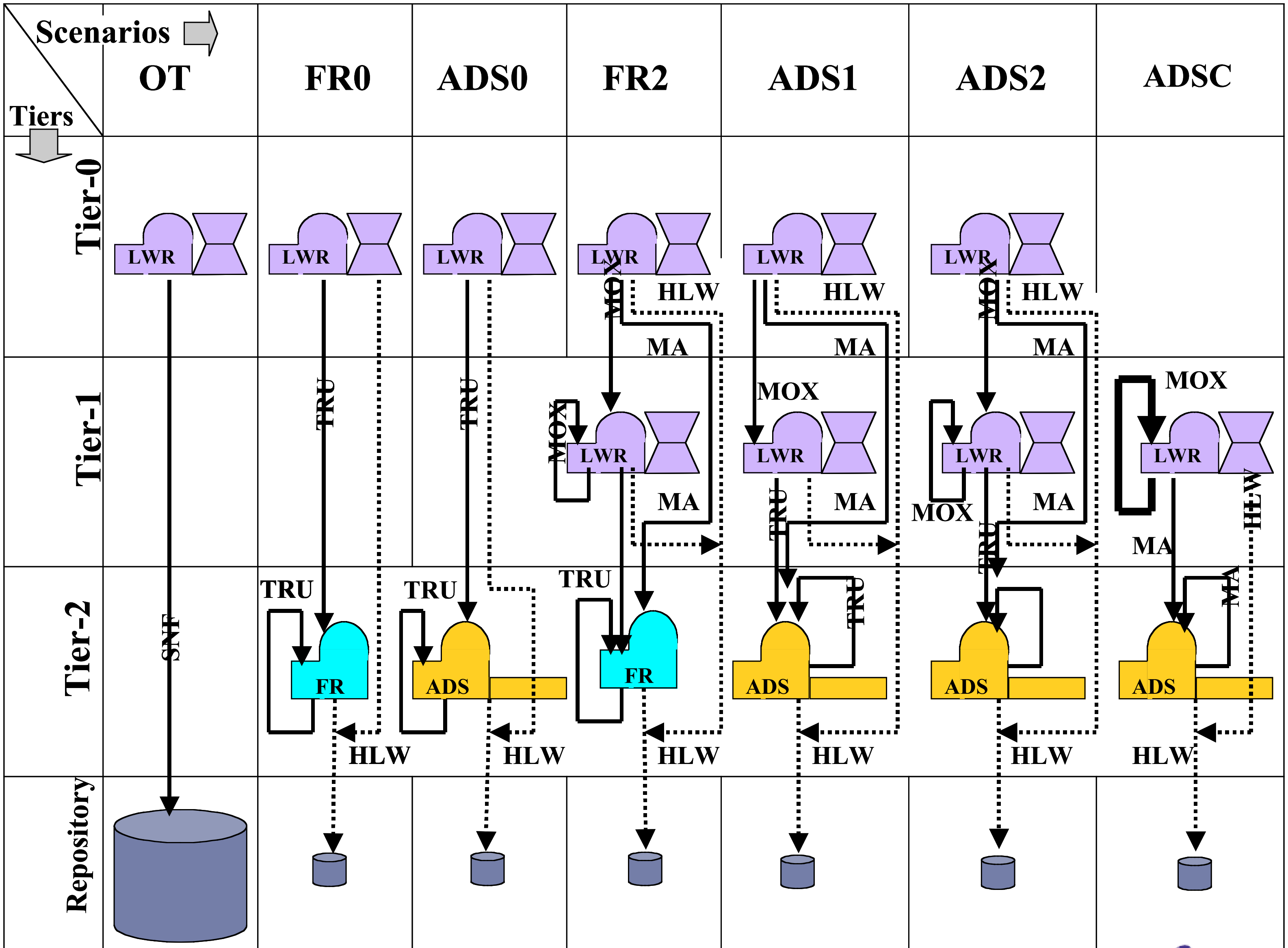
- Developed for OECD/NEA Study[b] and Modified for AAA Report-to-Congress Study[c];
- Scenarios focused on multi-tier configurations with once-through LWRs (Tier-0) feeding MOX-recycle LWRs (Tier-1) feeding a Fast-Spectrum Burner [FSB = Fast Reactor (FR) or Accelerator-Driven System (ADS)];
- Key metrics are cost (Cost of Electricity, COE), TRU waste mitigation; nuclear (materials) proliferation, and resource (natural uranium) utilization;
- "Top-Level" results guide the selection of scenarios for more-detailed dynamic (time-dependent) NFC analyses.

(a) R. A. Krakowski and C. G. Bathke, "Method for Quantitative Assessment of Cost and Proliferation Risks Associated with the Civilian Nuclear Fuel Cycle as Applied to the Advanced Accelerator Applications Program," Los Alamos National Laboratory document LA-UR-02-2369 (April 26, 2002).

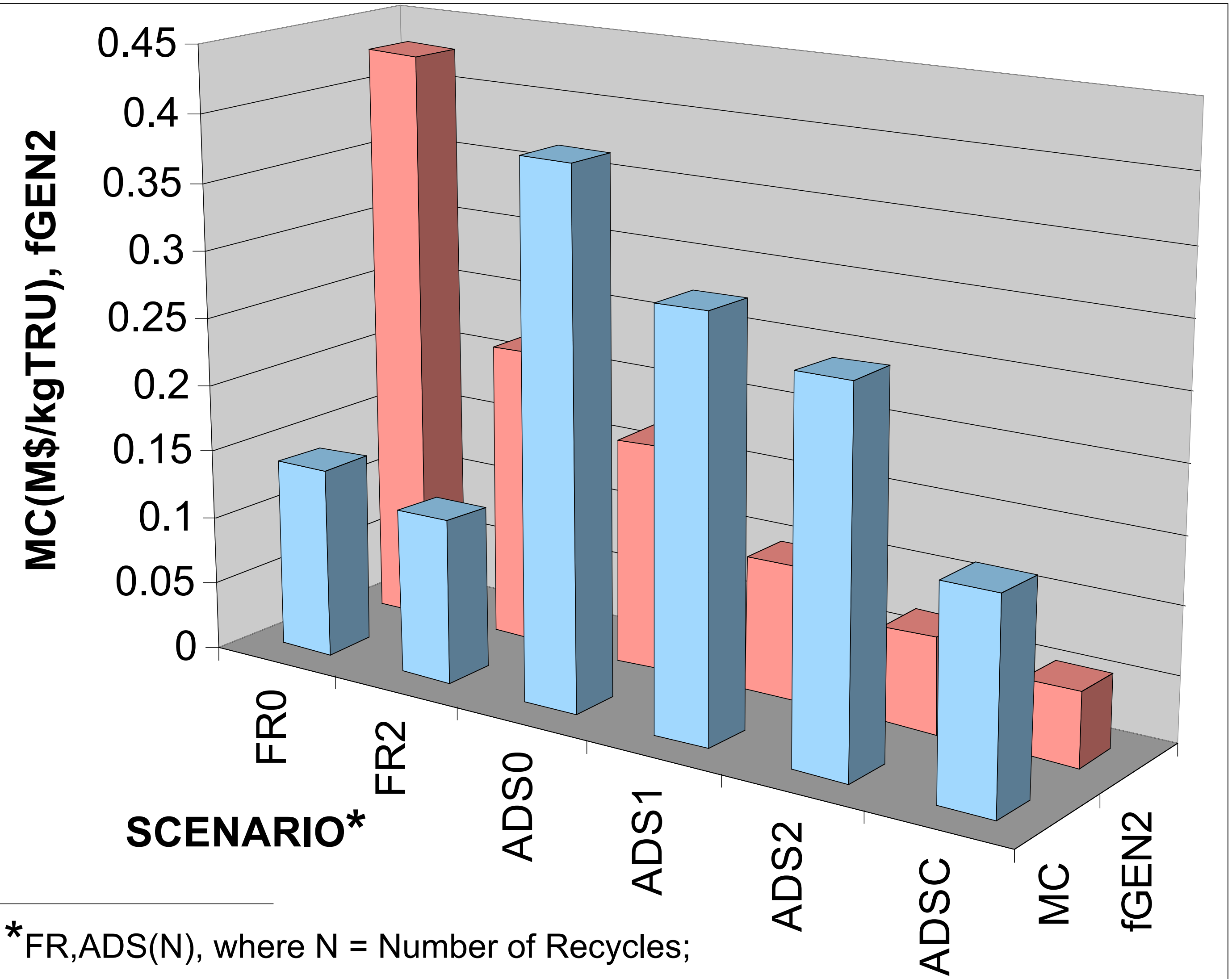
(b) P. Wydler (Chm.), "NEA-NDC Compartive Study of ADS and FR in Advanced Nuclear Fuel Cycles," OECD/NEA report (January 28, 2002, to be published).

(c) "Report fo Congress on the Advanced Accelerator Applicatiojns Program," U.S. Department of Energy document (May, 2002, in preparation).

Key Material Flows for the Seven AAA Nuclear Fuel Cycle (NFC) Scenarios Considered

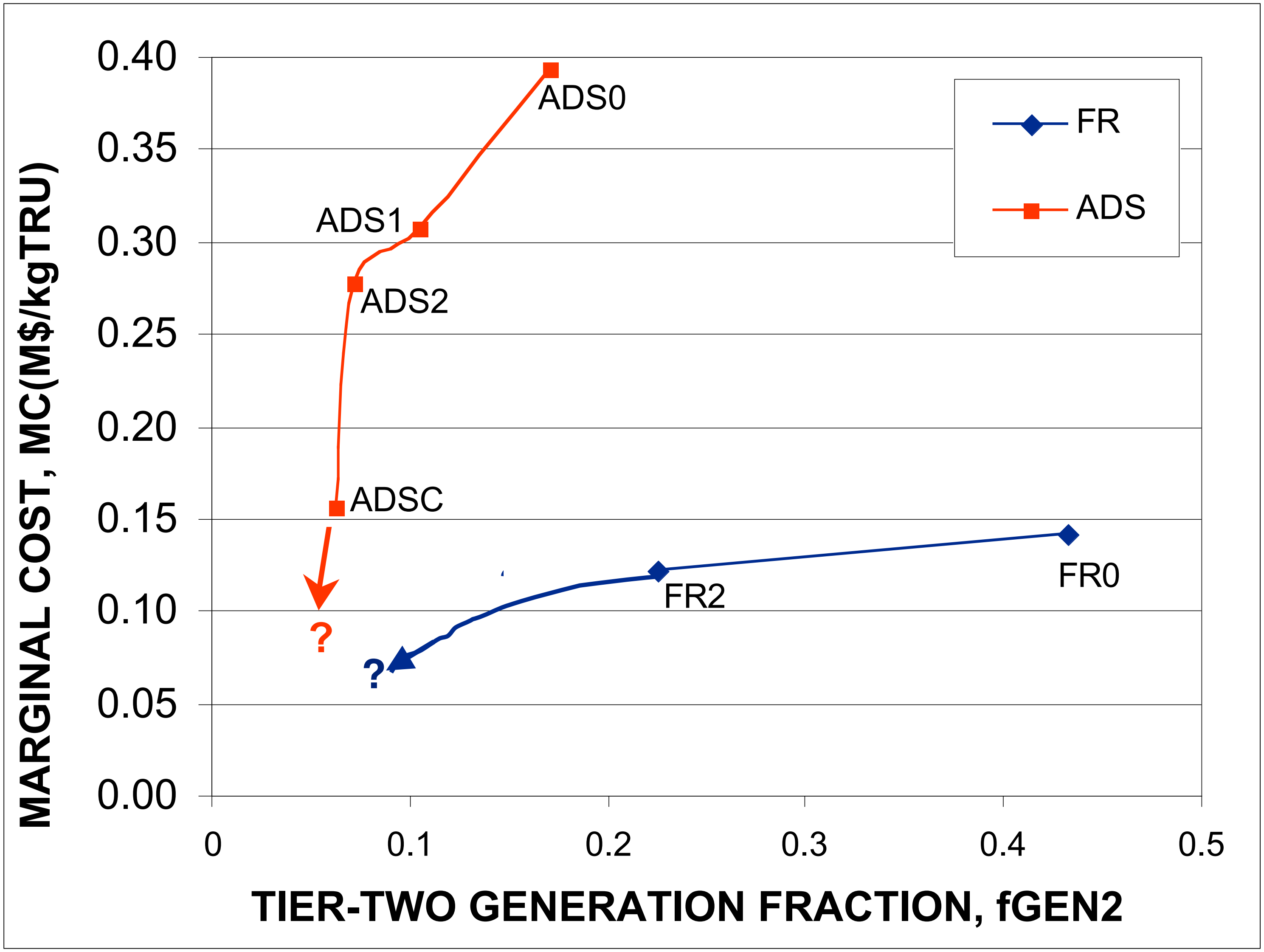


Lessons Learned from Equilibrium NFC Analyses: *Tier-1 Recycles Help ADS Cost and FR Support Ratios*

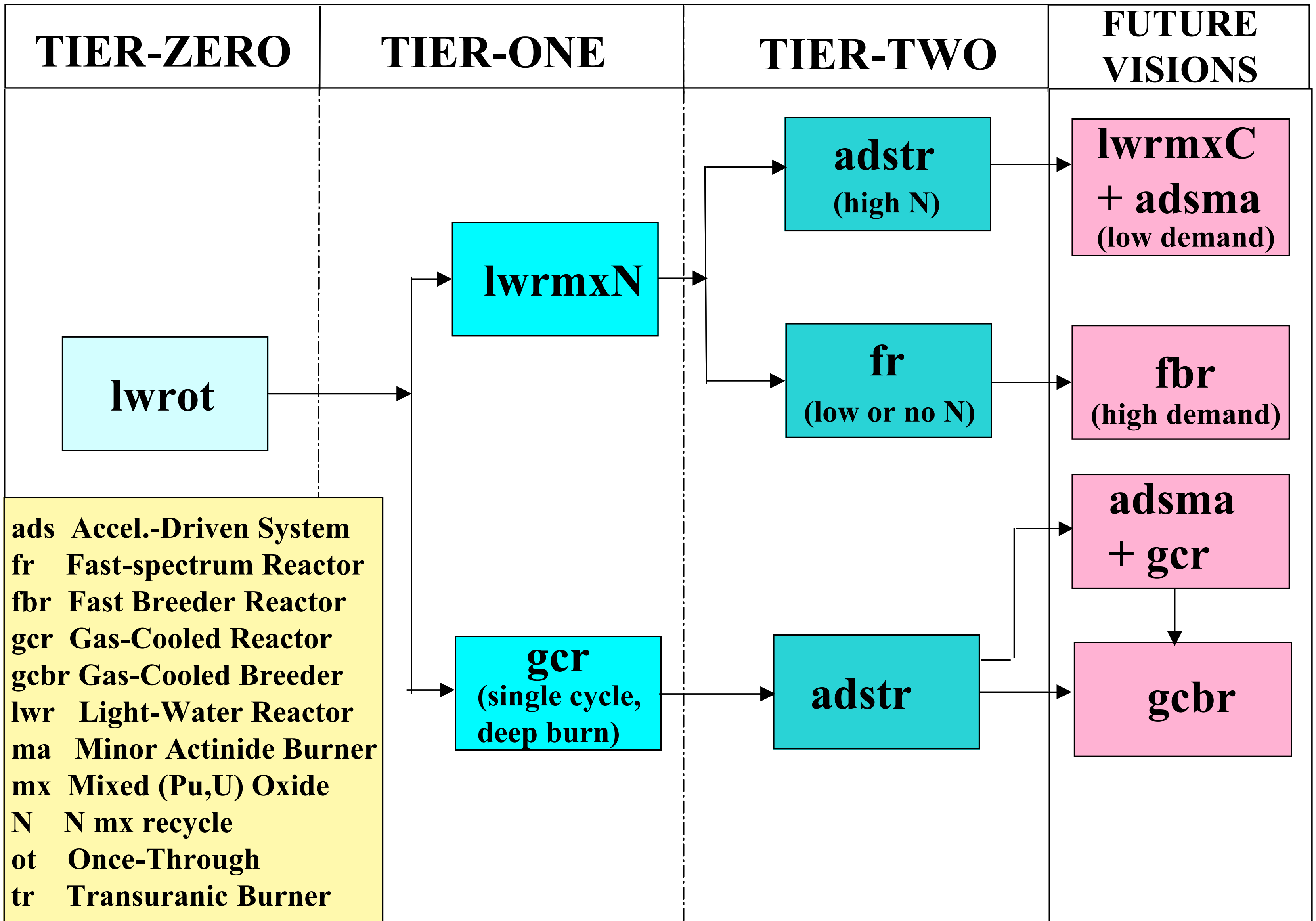


*FR,ADS(N), where N = Number of Recycles;
C = CORAIL (N ~7-8)

Lessons Learned from Equilibrium NFC Analyses: *Tier-1 Recycles Help ADS Cost and FR Support Ratios*



"Top-Level" Scenarios Suggested by AAARC Study and Under Consideration for Time-Dependent Analyses



"Top-Level" Scenarios Suggested by CEA/DOE Collaboration for Time-Dependent Analyses

nsc	Tier-0		Tier-1		Tier-2
1	*lwrot*	SNF →		~90/10 Pu/MA →	FSB (ADS, FR*)
2	*lwrot*	SNF →	*lwrmx(lr)* (2-3 recycle)	80/20 Pu/MA →	FSB (ADS*, FR*)
3	*lwrot*	SNF →	*lwrmx(hr)* (CORAIL, 8-10 recycle)	~1/99 Pu/MA →	FSB (ADS*, FR)
4	*lwrot*	SNF →	*htgr* (deep burn, 1 recycle)	~10/90 Pu/MA →	FSB (ADS*, FR)

lwrot once-through LWR
lwrmx(lr) low-recycle MOXed LWR
lwrmx(hr) high-recyle MOXed LWR
FSB fast spectrum burner
ADS accelerator-driven system
FR fast (critical) reactor

nsc scenario grouping
MA minor actinide
SNF spent nuclear fuel (*lwrot*)

* Preferred on the basis of equilibrium economics, except for *nsc* = 2, where within uncertainties both are equivalent.

Both *Simulation* and *Optimization* Models Are Being Explored as Means to Project Impacts of NFC Scenarios

- **Past efforts have focused on equilibrium (steady-state) NFC analyses (OECD, AAARC, LA-UR-02-2369);**
- **Two generic approaches to NFC dynamic modeling are being explored for AAA applications – *Simulation* and *Optimization;***

  - *Simulation Modeling*: NFCSim (Los Alamos development) and EXTEND™ (commercial process simulation tool from *Imagine That*!);

  - *Optimization Modeling*: FCOPT (Los Alamos development), with possible extension to MARKAL-US (IEA total energy optimization tool, *MARK*et *AL*location)

Simulation Models Are Used to Predict System Response to a Given Design Configuration

+ Response can be modeled with great accuracy and detail to identify possible costs, specified design or policy variables, *etc*.

+ Projects outcome of a single, specified set of design or policy variables;

– Generally simulations can not identify or narrow the search for optimal policies or designs;

+ Separate simulations are required for each design or policy alternative considered; set of such simulations can be used to scope out specific "design/tradeoff frontiers".

Optimization Models Provide Means to Reduce Number of Alternative Scenarios to be Simulated

+ Useful as a screening tool by searching the space for possible design variables to provide optimal designs and/or operating policies based on a (range of) single object function and set of constraints;
+ Sensitivity of optimal designs/policies can be examined *via* changes in both input parameters and systems constraints for a range of (single) object functions;
+ *Optimization Models* are typically extensions of *Simulation Models* that include unknown design and/or operating (decision) variables;
+ Describes and constrains the state of design/operating variables and gives relationships between costs and benefits for specific policy choices or restrictions;
+ Optimization Models, in addition to being used for screening of alternative design/policy choices, identify important data needs prior to extensive data collection needed to perform detailed simulations;

– Generally results from optimization models can be difficult to explain, requires more sophisticated interpretation; less control.

Dynamic Model/Modeling Priorities for Los Alamos NFC Systems Studies Task

- ***Simulation Models*** **will lead dynamic NFC analyses with NFCSim representing the lead effort, which will be supported/augmented/QA'd by EXTEND™;**

- ***Optimization Models*** **will be pursued as a second priority, with the NFC-specific FCOPT model being adapted to AAA needs and approaches (multi-tiered NFC scenarios);**

- **Integration/commonality/basing/*etc*. of efforts in all three modeling efforts is a watchword of overall activity:**

  - between/among dynamic NFC Simulation and Optimization Modeling activities;

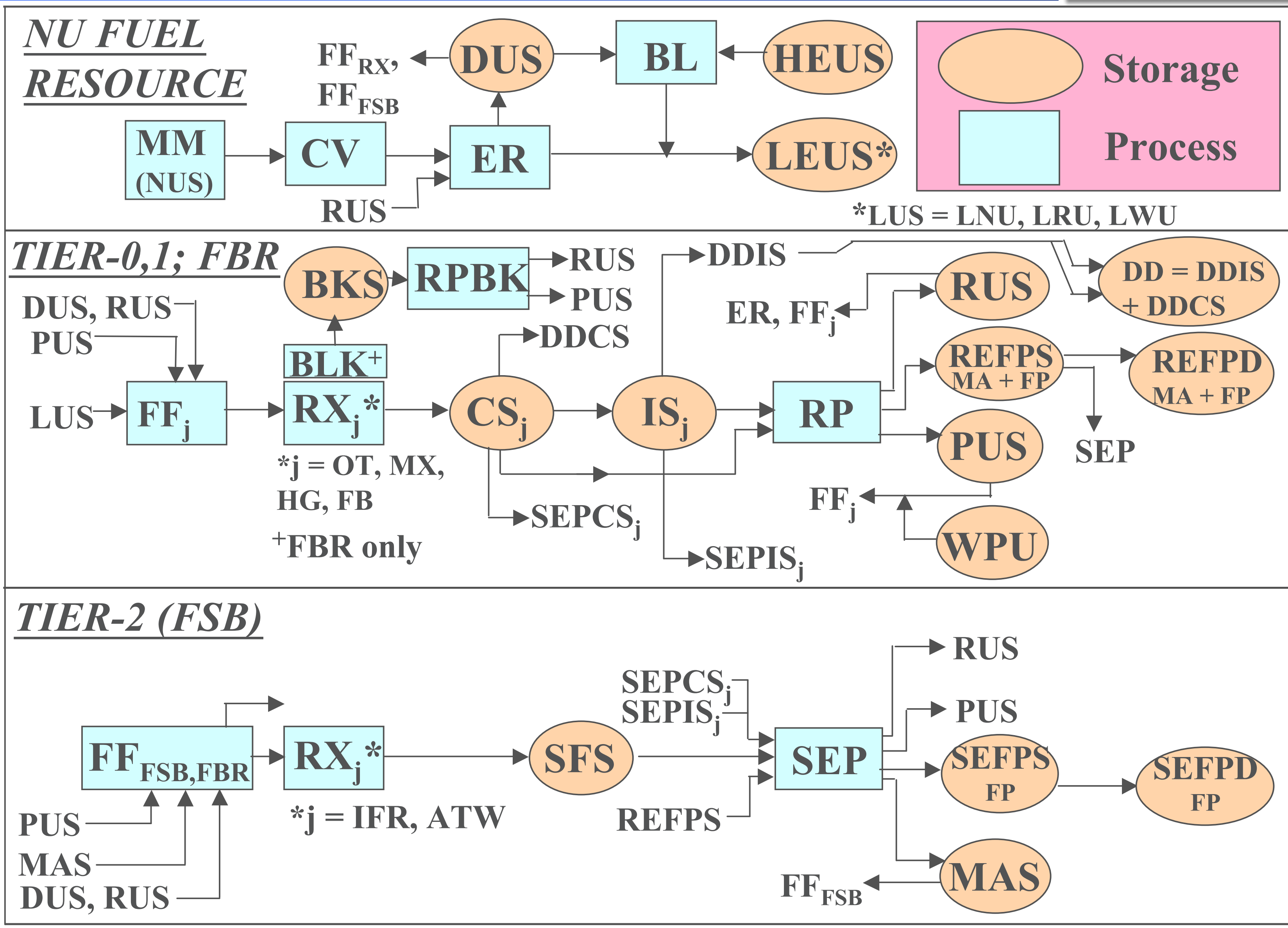
  - between dynamic NFC modeling and neutronics modeling;

  - between dynamic NFC modeling and all processing activities;

Structure of a Linear Programming (LP) Problem

- ***Objective***: **an LP is designed to find the best or 'optimal' solution (*e.g.*, best combination of processes) – life-cycle cost; minimum repository impact; minimum operational worker radiation dose; minimum proliferation risk (as defined by a range of criteria); *etc*.**
- **Activities or Decision Variables: alternatives that give what to do, how to do it, and how much of it to do to minimize or maximize a given Objective (function); in the context of FCOPT, these are inventories or flow rates, *x(m,p,t),* or electricity generation rates, *gen(p,t),* for given sets of materials {*m*}, processes {*p*}, and times {*t*};**
- **Constraints: specifies the conditions under which combinations of Activities can be selected – overall demand rates; technology deployment rates; storage or processing capacity limits; material availability; Exogenous Technical Learning (ETL) impacts on cost and deployment, *etc*.**

Mass Flows in NFC Optimization Model FCOPT



Mass and Process Notation Used in NFC Optimization Model FCOPT

NU Fuel Resource Processes, p	
BL	^{235}U-^{238}U Blending
CV	U_3O_8 - UF_6 Conversion
DUS	Depleted Uranium Storage
ER	235U Enrichment
HEUS	Weapons-Grade Uranium
LEUS	LEU Supply
MM	Mining and Milling
DUS	Depleted Uranium Storage
NUS	Natural Uranium Storage

TIER-0,1, FBR Processes, p	
BLK	(FBR) Blanket
BKS	Storage for Irradiated FBR Blanket Material
CS_j	SNF Cooling Storage for Reactor j
DD	Direct Disposal SNF Repository, (DDCS + DDIS)
DDCS	Direct Disposal SNF Repository from CS
DDIS	Direct Disposal SNF Repository from IS
FF_j	Fuel Fabrication for Reactor j
IS_j	SNF Interim Storage for Reactor j
MAS	MA Storage
PUS	Separated Pu Storage
REFPD	Repository Disposal from REFPS
REFPS	(FP,MA) Storage from Reprocessing
RP	Reprocessing [U, Pu (MA,FP) Separation]
RPBKS	Reprocessing of BKS Materials
RX_j	Reactor/Irradiator j
ADS	Accelerator-Driven System
FBR	Fast-Spectrum Breeder Reactor
FSB	Fast-Spectrum Burner (ADS, FR)
HG	High-Temperatur Gas-Cooled Reactor
IFR	Integral Fast Reactor, IFR
MX	MOX LWR
OT	Once-Through LWR
SEFPD	Repository Disposal from SEFPS
SEFPS	Storage of FP from SEP
SEP	Separations [U, Pu, MA, FP]
SFS	Spent-Fuel Storage for Tier-2 Operations
WPS	Weapons-Grade Plutonium Storage

Mass and Power Balance:

$$\sum_{\{m\},\{p\}} a(m,p) * x(m,p,t) \geq b(t)$$

Objective Function:

$$\min \left[\sum_{m,p,t} UC(p) * x(m,p,t) / (1+r)^t \right]$$

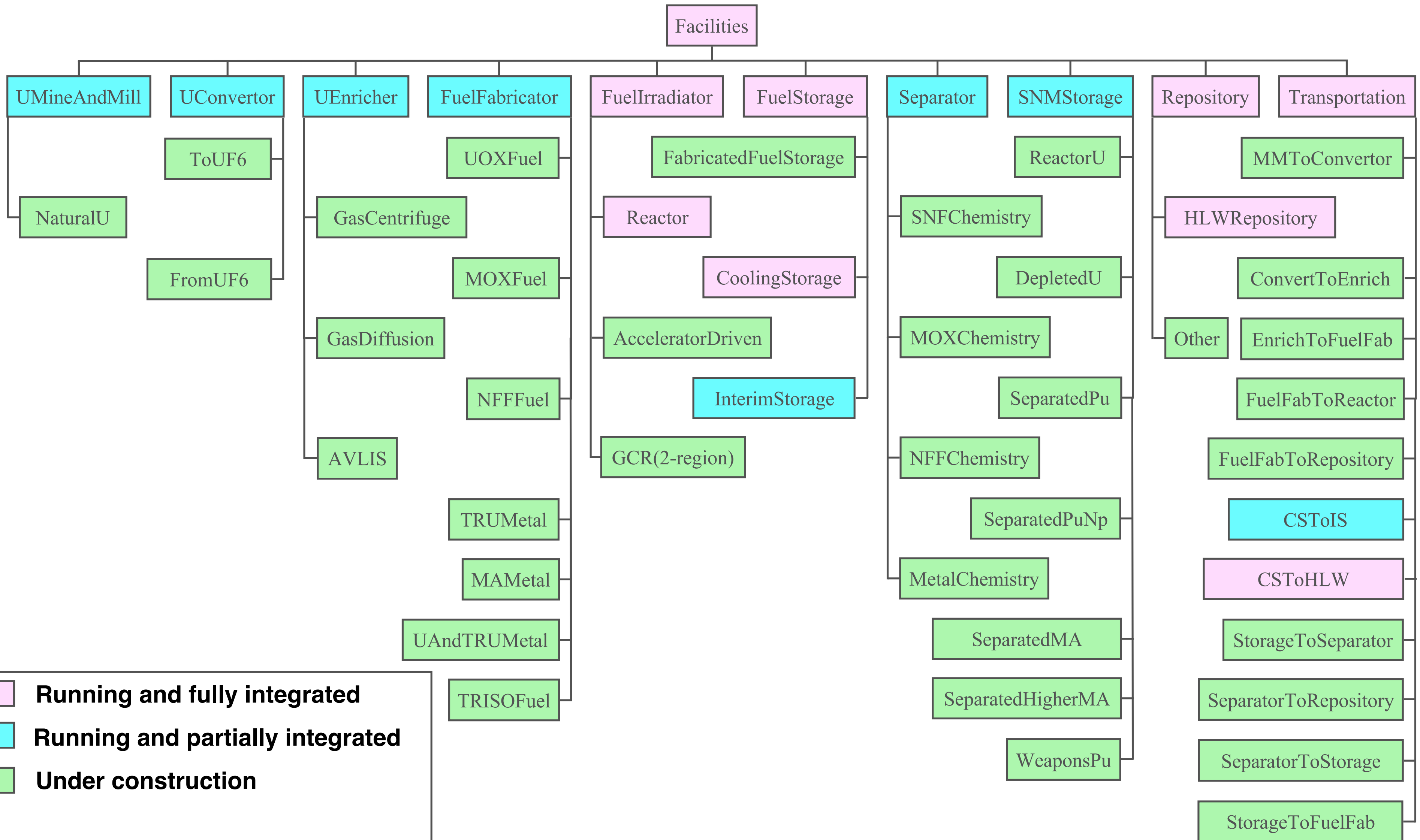
Materials, m	
BMX	(FBR) Blanket-Generated MOX
DU	^{235}U-Depleted Uranium
FP	Fission Products (LLFP + SLFP)
LEU	Low-Enriched Uranium
LNU	LEU from Natural Uranium
LRU	LEU from Reactor (exposed) Uranium
LWU	LEU from Weapons-Grade Uranium
NU	Natural Uranium
LFP	Long-Lived Fission Products
MA	Minor Actinides
MOX	(fresh) Mixed (U,Pu) Oxide Fuel
NU	Natural Uranium
RHTG	SNF from RXHG
RGBR	SNF from RXFB
RMX	Spent MOX Fuel
RPU	Reactor-Grade Plutonium
RU	Reactor(exposed) Uranium
RUX	Spent UOX Fuel
SFP	Short-Lived Fission Products
SNF	Spent Nuclear Fuel
WPU	Weapons-Grade Plutonium

NFCSim Models the Flow of Nuclear Materials Through the Nuclear Fuel Cycle

- NFCSim tracks mass flow at the level of discrete reactor fuel loadings/discharges, logging in time:
  - isotopic distribution;
  - originating reactor;
  - arrival and departures dates.
- Minimal time step is one day:
  - event durations expressed as an integer number of days;
  - simulation proceeds sequentially from event to event.
- Costs will be tracked similar to the "DELTA" model:
  - system-wide Cost of Electricity;
  - discounted Life-Cycle Cost (LCC) a new feature.
- Residence times of isotopes of interest are recorded for possible use in proliferation-resistance model.
- Simulation begins with present-day US fleet of commercial nuclear reactors (IAEA, EIA).

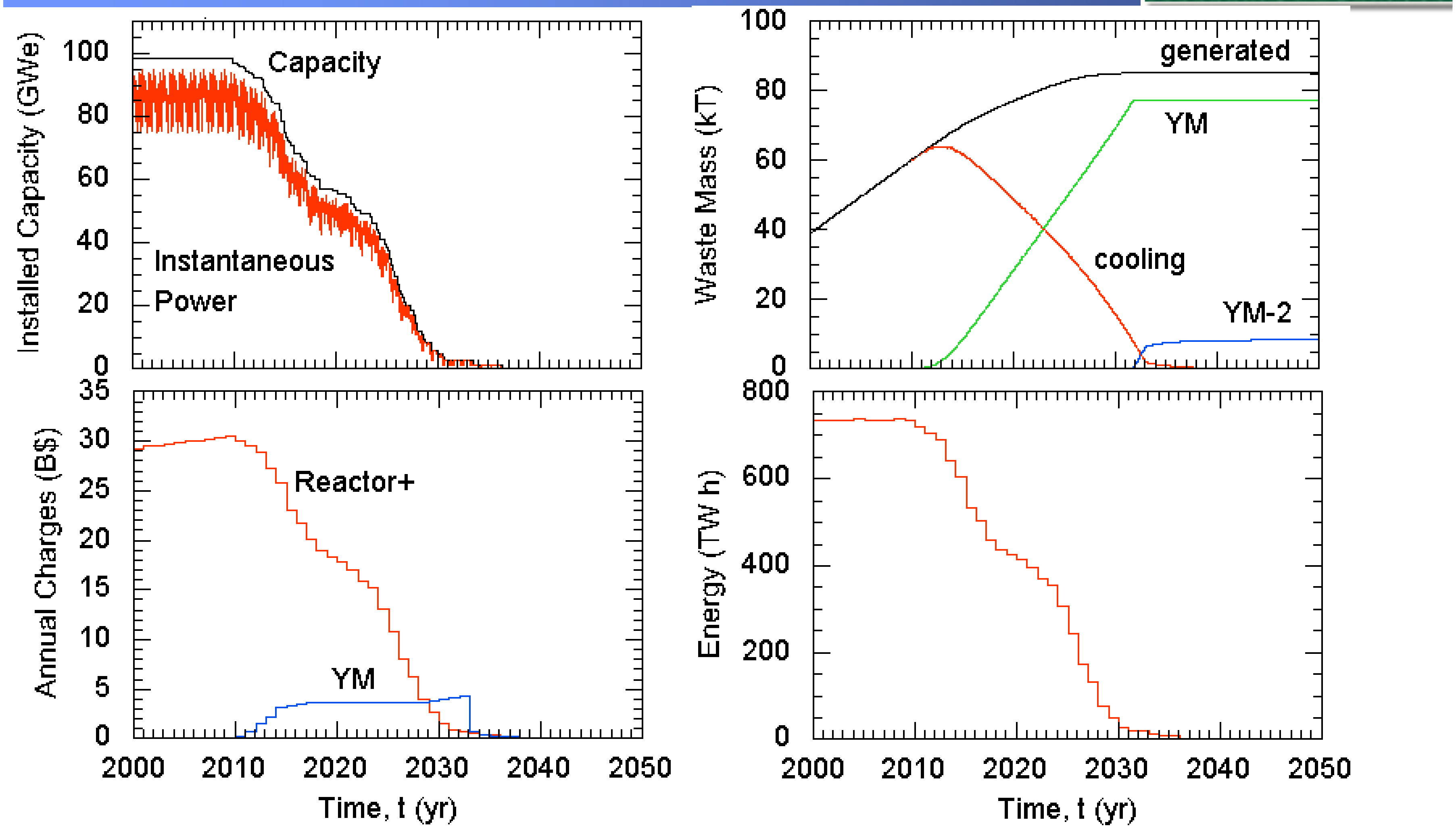
A More Detailed Class Structure for Facilities Modeled in the NFCSim Model

Advanced Accelerator Applicatio



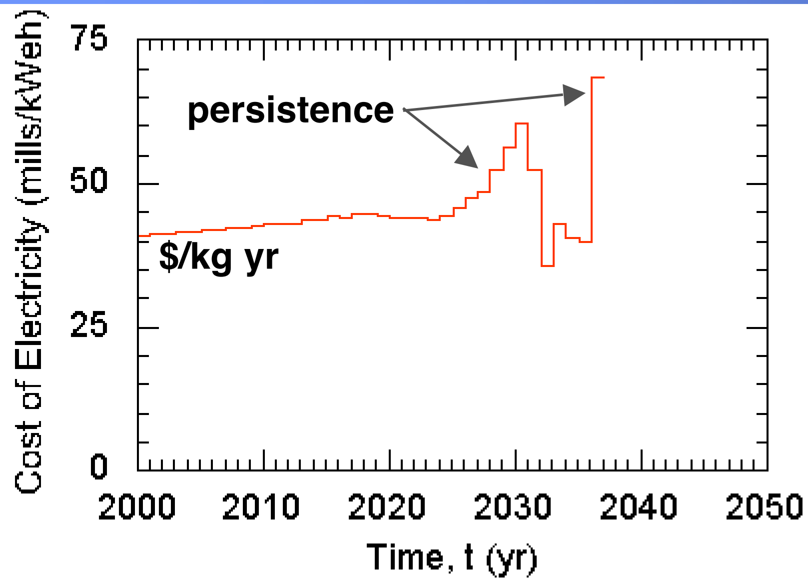
- Running and fully integrated
- Running and partially integrated
- Under construction

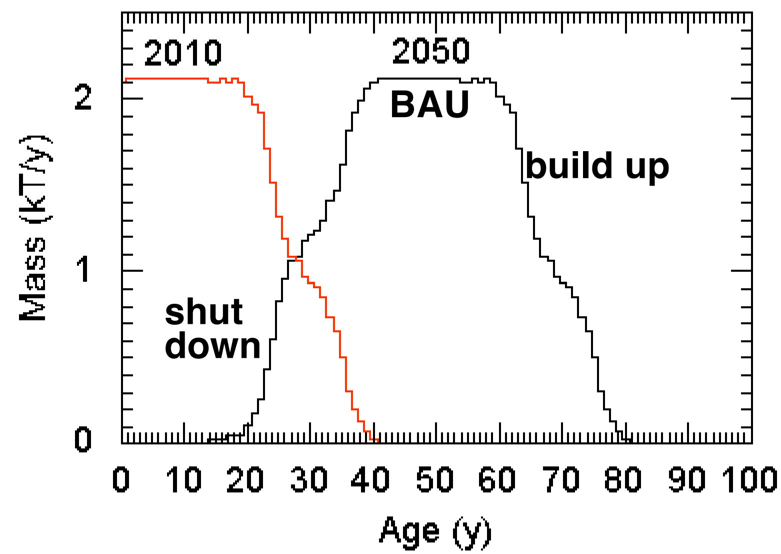
Sample Results Generated from Current Version of NFCSim



- Only the commercial nuclear fleet is modeled (*I.e.,* nuclear phase out).
- Reactor cycle is 312 days at full power and 53 days down (85% plant factor).
- Burn-up is 40 MWt d/kgIHM, which corresponds to ~ 4% IHM fission fraction.

Sample Results Generated from Current Version of NFCSim (cont.-1)





- Plant life is assumed to be 40 years, without license extension; no new construction;
- SNF must be 7 years old before it is moved from cooling storage.
- Equilibrium (DELTA model) costing is presently used and includes costs for:
  - reactor [use of unit capital cost, UTC($/We) and a fixed charge rate, FCR(1/yr)]
  - O&M and D&D taken as annual pay rate (1/yr) as fraction of total capital cost;
  - cooling storage [UC_{CS}($/kgHM/yr)];
  - transportation [UC_{TR}($/kgHM)];
  - repository cost corresponds 1 mill/kWe h (equivalent to 327 $/kgIHM).
- Time-dependent cost issues remain to be addressed, *e.g.*:
  - capitalization of all (reactor, storage, fabrication, processing, *etc.*) costs;
  - $/kg yr unit costs (*e.g.*, for cooling storage) are not realistic;
  - persistence, *e.g.*, who pays for cooling storage after shutdown?

Simulation Modeling using EXTEND™

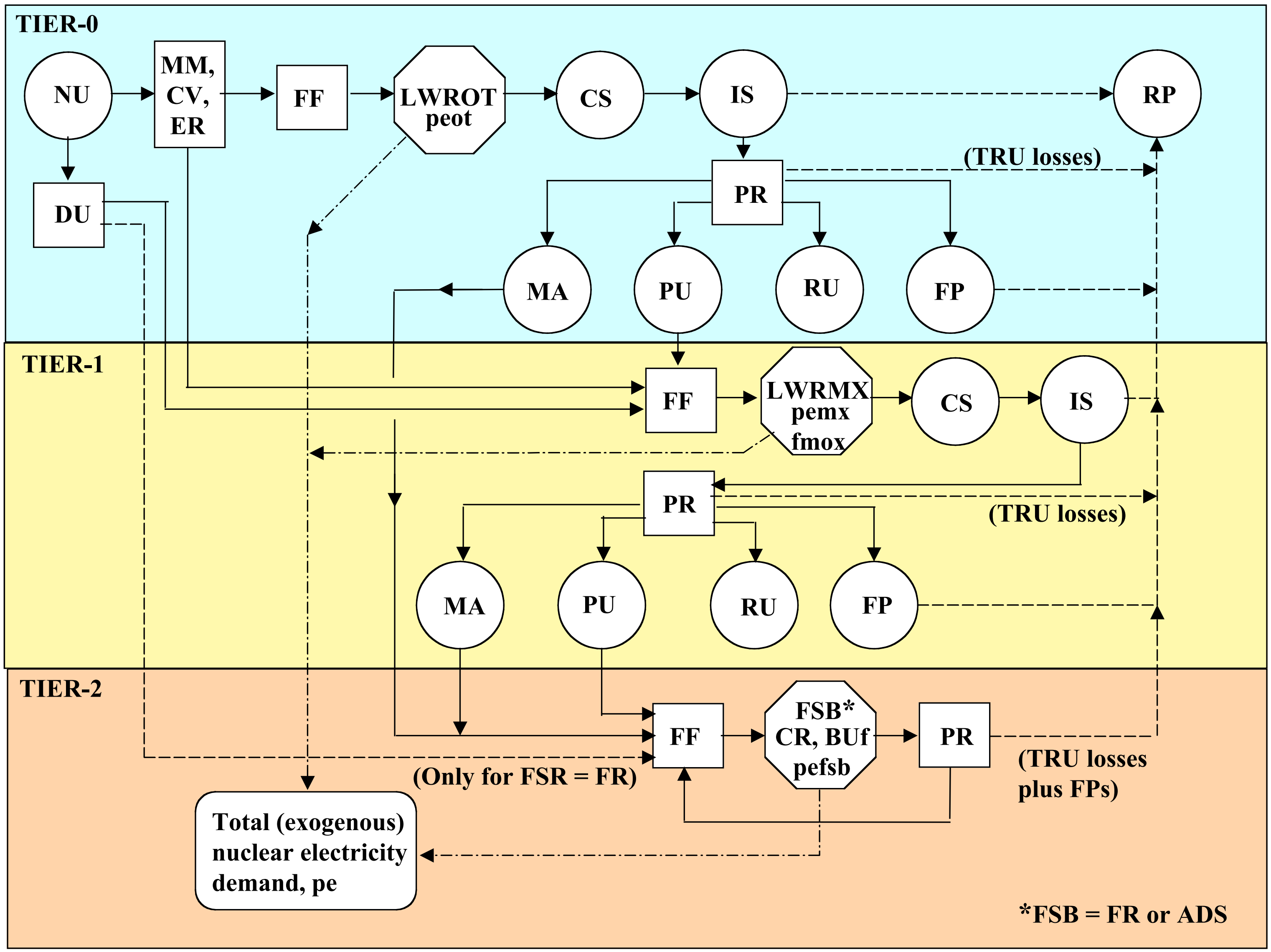
- **EXTEND™ is a commercial simulation software package (*Imagine That!*) that can simulate both continuous or discrete events (for dynamic NFC modeling in the long term, continuous simulation will be used).**

- **Features of EXTEND™:**
  - **"Building Block" (graphical) approach using pre-programmed modules and graphical user interface (GUI) permits rapid model construction and evaluation:**
  - **Hierarchical decomposition facilitates construction and understanding of even complex systems[a] ;**

    [a] For example, a complex SNF reprocessing plant can be modeled, then collapsed into a "black box" to avoid visual clutter when used in a simulation with other "black boxes" that model reactors, fuel-fabrication plants, waste treatment facilities, *etc.*
  - **Plotting, file storage, etc. is built-in; direct input/output connection to spreadsheet; ultimately.**
  - **Supports optimization (*via* multiple simulations), Monte Carlo, sensitivity analyses, costing, *etc*.**

General (Preliminary, Simplified) Structure of Three-Tiered NFC Being Modeled by EXTEND™

Advanced Accelerator Applicatio



Description of Exogenous Drivers in EXTEND™ NFC Model

❋ Total (capacity) demand, *pe*: exogenous growth at rate *grate*, with $pe = peo*(1 + grate)^t$;

❋ Generation capacity conservation: $pe = peot + pemx + pefbs$;

❋ MOX-capable LWR capacity: *pemx* exogenously introduced *via* logistic function, with limit being $pe - pefsb$;

❋ UOX *versus* MOX capacity: $peott = peot + pemx*(1 - fmox)$ and $pemxt = pemx*fmox$;

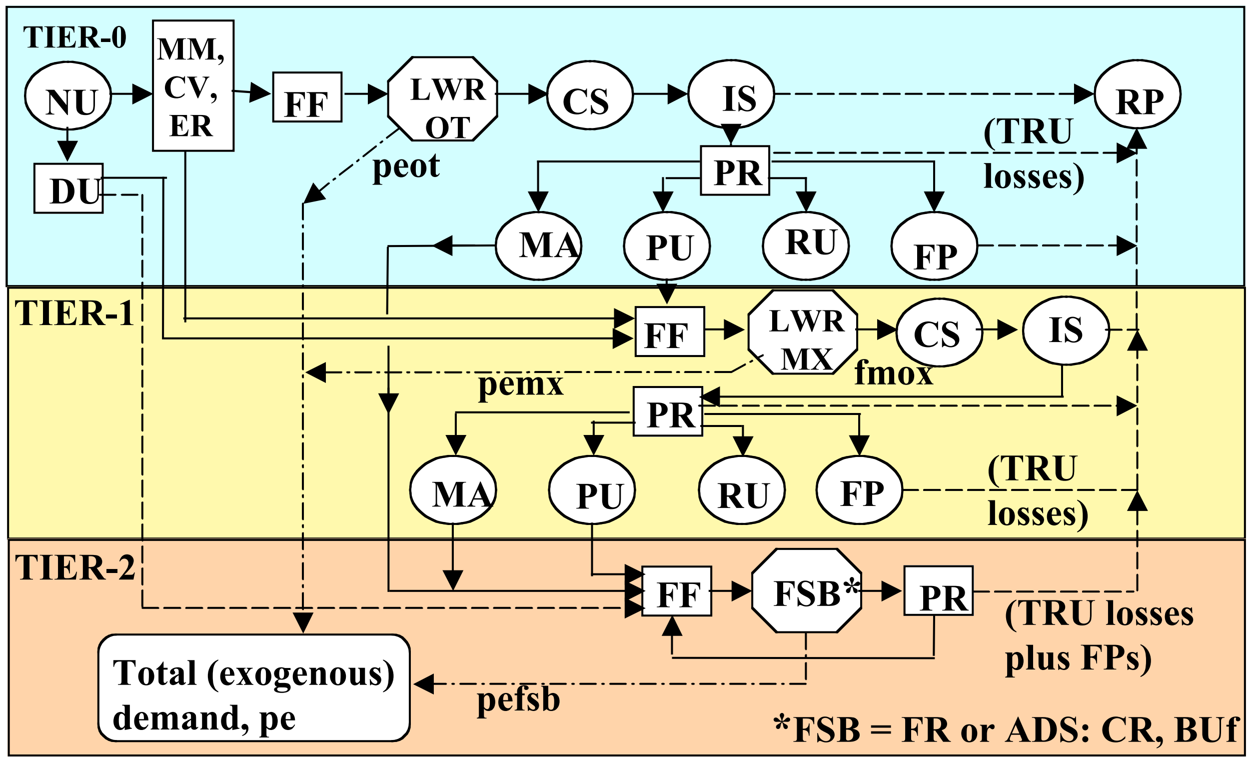
❋ CS →IS SNF transfer (Tier-0,1): *tcool* period in CS, then transfer to IS;

❋ IS → PR transfer (Tier-0): allocate based on fraction of IS inventory and separated-Pu level;

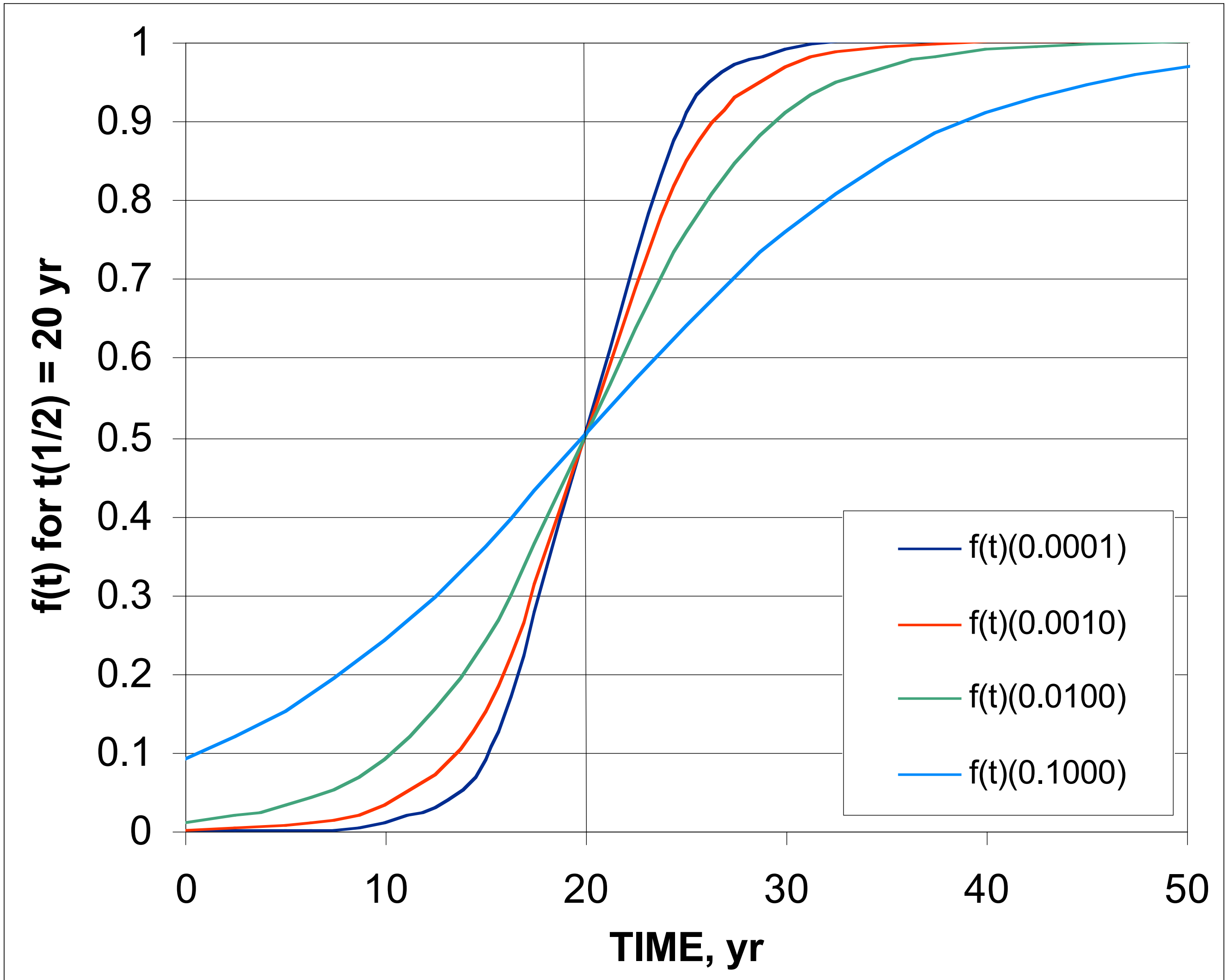
❋Fraction MOX, *fmox*: set to maximum value *fmoxo* if separated-Pu (Tier-0) is above minimum level; decreased if separated-Pu (Tier-0) inventory falls below minimum level;

❋ FSB (Tier-2) fueled from Tier-0,1 MA storage and Tier-1 separated-Pu storage;

❋ Rate of (Tier-2) FSB capacity introduction: exogenous deployment driven by logistic (function) increase in rate of (Tier-2) fuel fabrication.



Logistics Function Presently Used to 'Exogenize' the Endogenous



$$f(a,b,t) = \frac{ae^{b}}{1+a}$$

$$f_t = bf(1 - f)$$

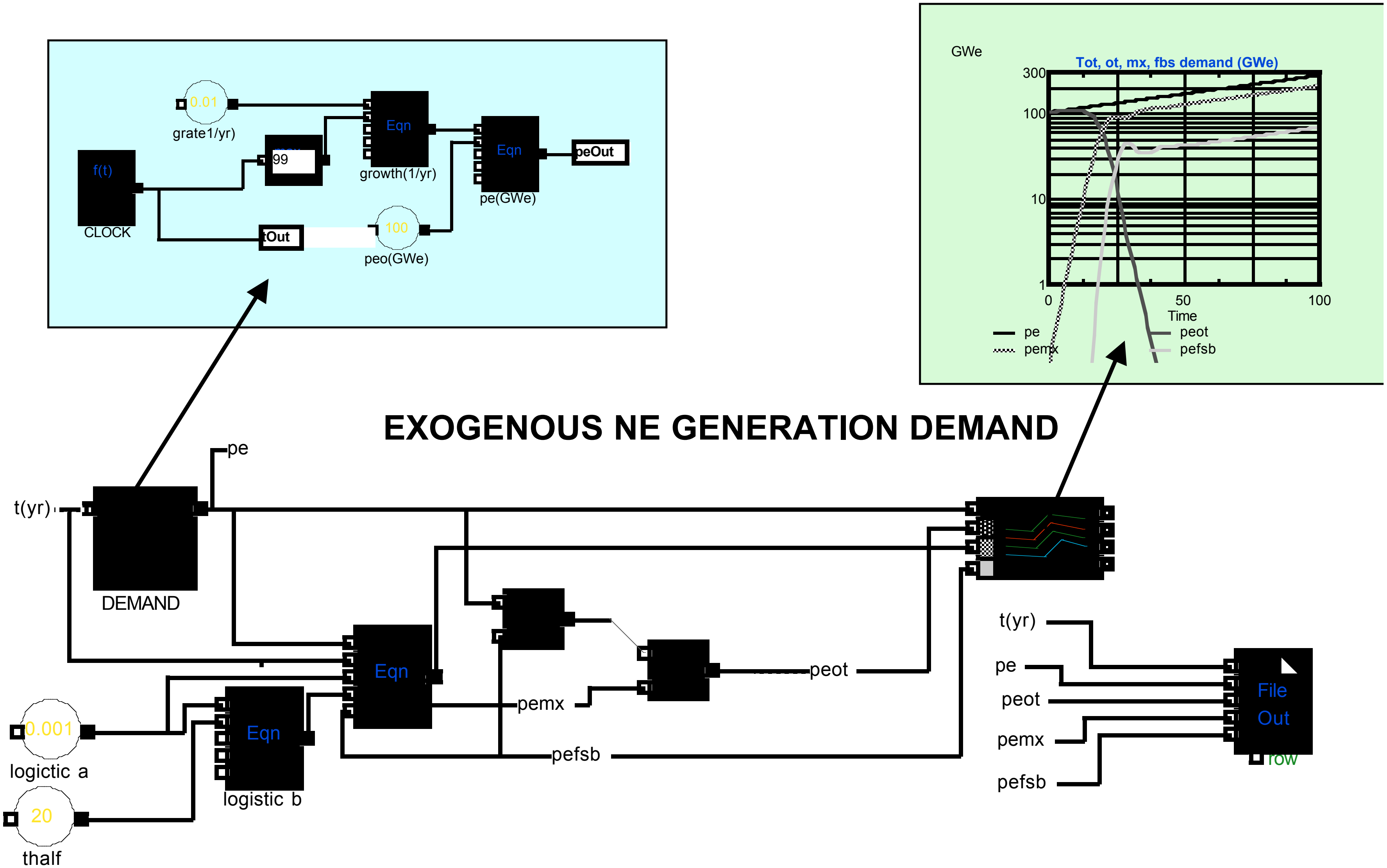
$$f_t(0) = \frac{ab}{(1+a)^2}$$

$$t_{1/2} = \frac{\ln(1/a)}{b}$$

$$MS(t) = MS_f\, f(a,b,t)$$

Demand Portion of EXTEND^{T} NFC Model

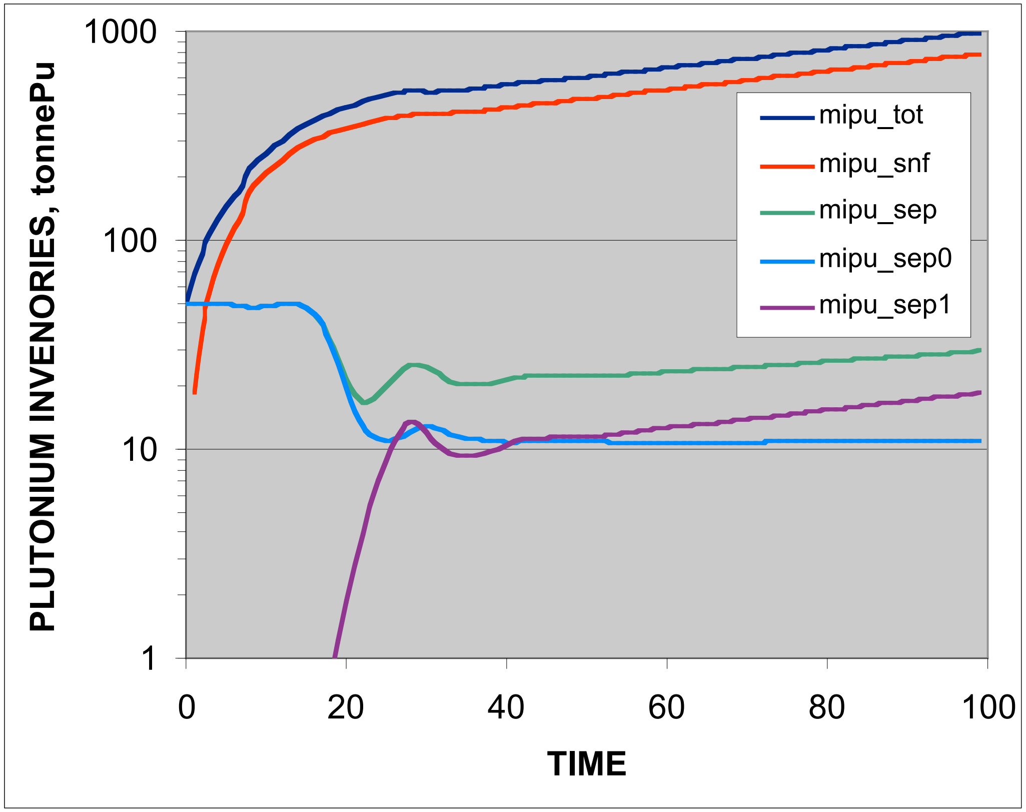
Advanced Accelerator Applicatio



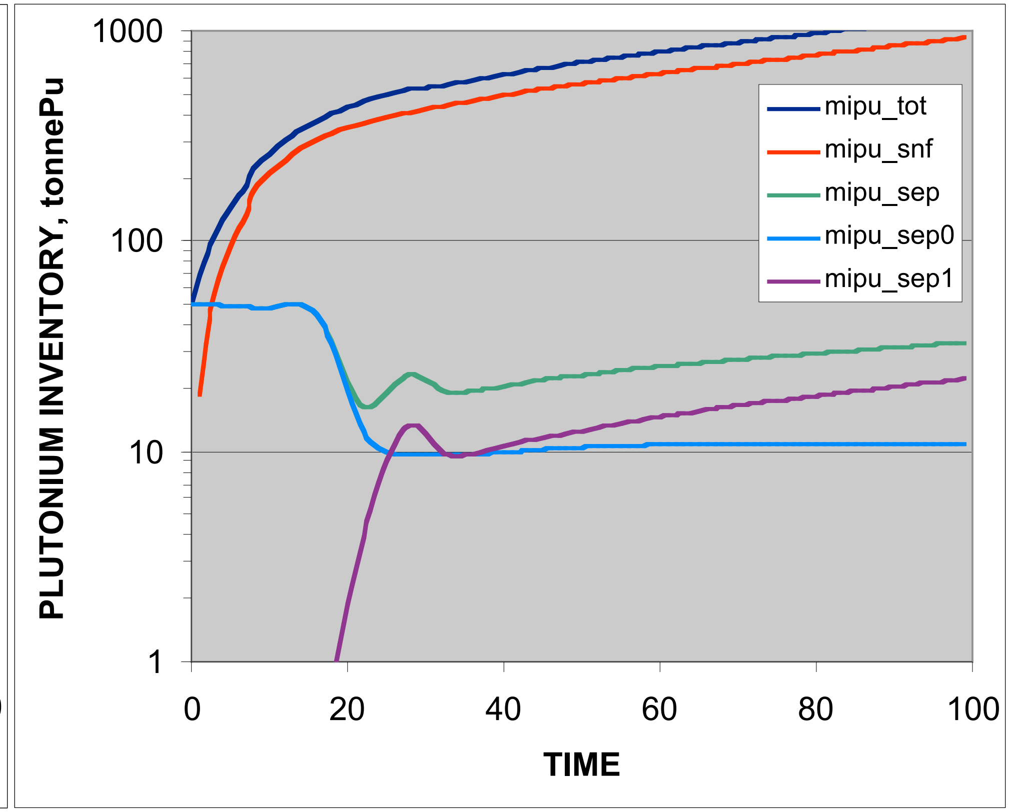
EXTEND™ Example: ADS or FR Tier-2; Pu Inventories

Advanced Accelerator Applicatio

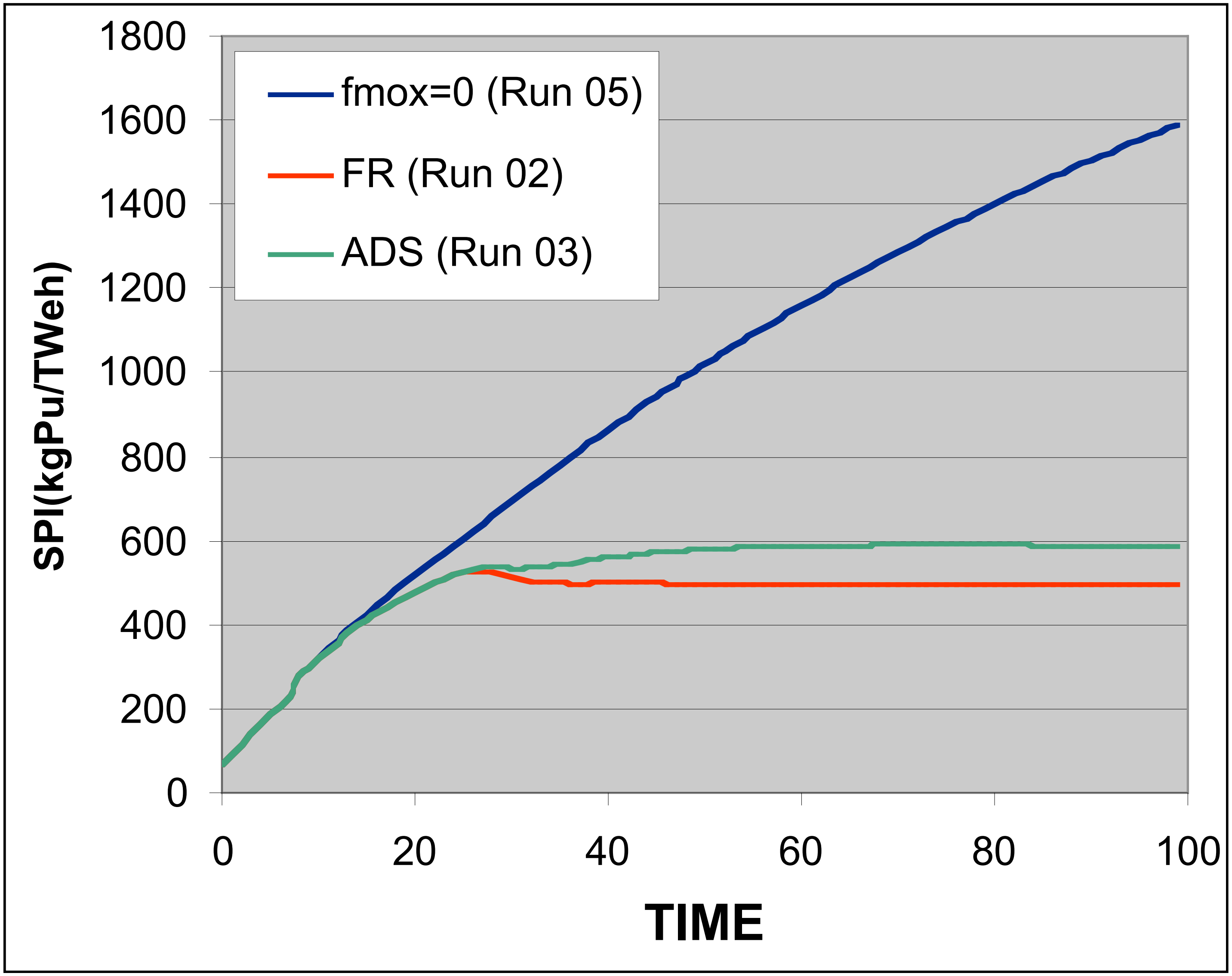
FR Tier-2



ADS Tier-2



EXTEND™ Example: ADS or FR Tier-2; Specific Pu Inventories



EXTEND^{TM} Model: Ongoing/Planned Development

- **Include all significant processes, in close parallel with NFC*Sim* simulation and FCOPT optimization models:**
  - Reactors;
  - Cooling/storage (retrievable);
  - Reprocessing;
  - Fuel fabrication;
  - Repository;
  - Waste streams (HLW, ILW, LLW);
  - Electricity production;
  - Uranium requirements (Mining, milling, conversion, enrichment);

- **Use appropriate detail (can be enhanced at later date):**
  - Mass balances (isotopic including U, Pu and MA, selected FPs);
  - Energy balance to meet exogenous demand for nuclear energy;

- **Treat processes as "Continuous" where appropriate for the time lines being explored;**

EXTEND^{TM} Model: Ongoing/Planned Development (cont.-1)

- **Couple model input more tightly with neutronics computations (mass fractions, isotopics, *etc*.);**

- **Advance/increase model fidelity at all tiers (isotopics, recycle, loss streams, process delays, in-reactor inventories, *etc.)***

- **Add in economic and proliferation metrics;**

- **Enhance "user friendliness (Spreadsheet-based input and output, including graphics;**

- **Integrate/normalize results from *simulation* models with results from *optimization* Model.**

FCOPT, NFCSim, and EXTEND™ Models Following "Top-Level" Processes in the Nuclear Fuel Cycle

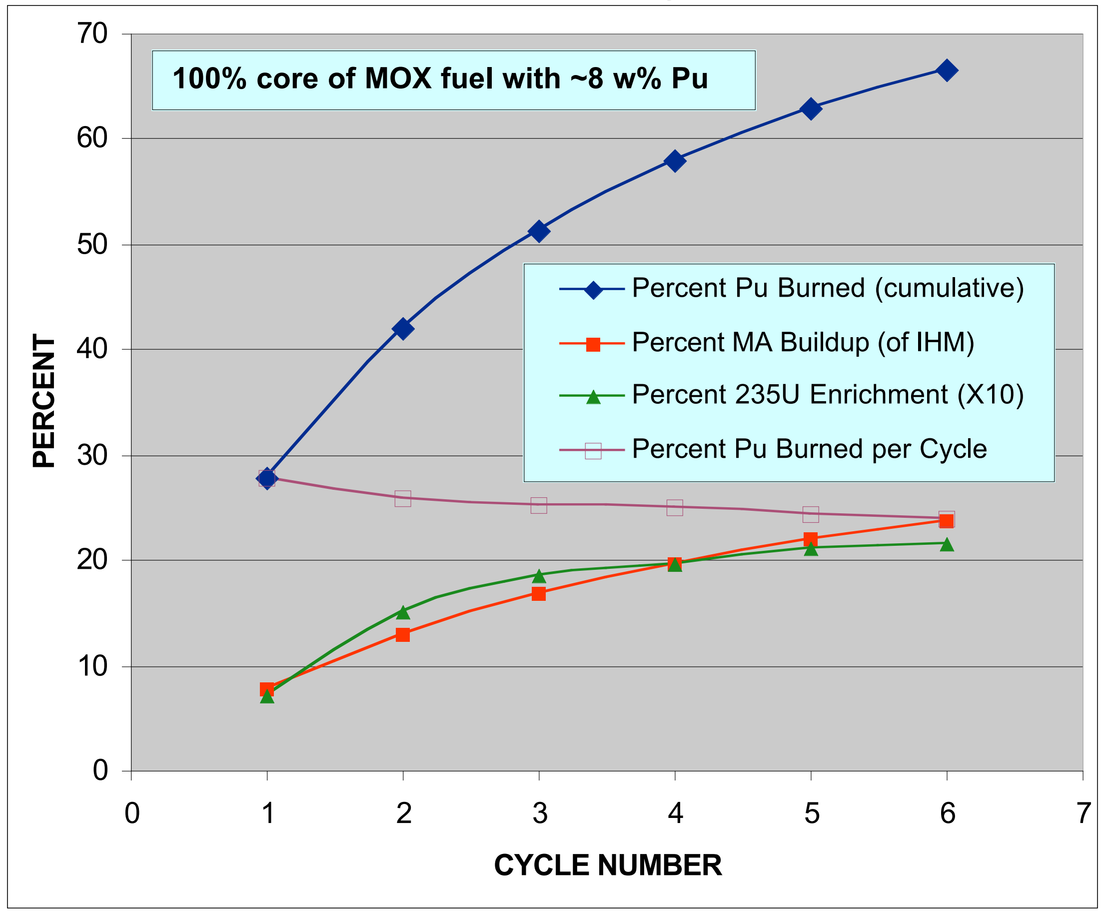
Models:	Simulation		Optimization
Process	EXTEND	NFCSim	FCOPT
Mining and Milling	X	X	X
Conversion	X	X	X
Enrichment	X	X	X
Fuel Fabrication	X	X	X
Reactor	X	X	X
Storage	X	X	X
Processing	X	X	X
Repository	X	X	X
Transportation	X	X	
Weapons HEU Blending			X
Weapons Pu Disposition			X

Neutronics Support of Systems Studies

Advanced Accelerator Applicatio

- Basic irradiation calculations performed for multi-recycle of Pu from SNF(re: adjacent figure);
- Detailed 1/8 core model of LWR developed and safety calculations using MOX fuel confirmed (for additional multi-recycle (MIX) calculations)
- Future / On-going Activities:
  - Couple neutronics calculations with NFCSym;
  - Database composition of all US SNF for NFCSym;
  - Burns with increased ^{90}Sr and ^{137}Cs content to maintain SNF standard, even for ‘fresh’ MOX.

Multi-Recycle of Pu in LWRs with MIX Core Configurations



Front-end Repository Impacts: Key Components of Spent Nuclear Fuel As Related to Repository Thermal Impacts

ACTINIDES

SPENT NUCLEAR FUEL **SNF**

CLADDING **CLD**

URANIUM **U**

PLUTONIUM **PU**

MINOR ACTINIDES **MA**

FISSION PRODUCTS **FP**

NON-VOLATILE FISSION PRODUCTS **NVFP**

VOLATILE FISSION PRODUCTS **VFP**

VERY LOW HEAT RADIONUCLIDES **VLHR**

HIGH HEAT RADIONUCLIDES **HHR**

LOW HEAT RADIONUCLIDES **LHR**

Notes:

MA = Np, Am, Cm

VFP = Inert Gases (He, Ne, Ar, Kr, Ze, Rn) + Halogens (F, Cl, Br, I)

HHR = ^{90}Sr + ^{137}Cs (but all isotopes)

VLHR = FP – VFP – HHR

LHR = VLHR + MA (possibly Pu)

SNF, VLHR, HHR, and LHR represents notation taken from from:
C. W. Forsberg, Nucl. Technol., 131(8), 252 (2000).

"Tier-less" Front-end Scenarios for Investigating Repository Impacts

Scenario, *nsc*	Short Description[c]	Elaborated Description[a]
1	Base Case	Direct disposal of SNF fuel assemblies
2	1 – U(ranium)	Vitrified [MA + Pu + NVFP]
3	2 – {Cs,Sr}	Vitrified [MA + Pu + VLHR = LHR][b]
4	3 - Pu	Vitrified [1 - U - HHR - Pu = MA + VLHR = LHR][b]
5	2 - Pu	Vitrified [1 - U - Pu = MA + NVFP][b]
6	4 - MA	Vitrified [1 - U – HHR - Pu – MA = VLHR][b]
7	5 - MA	Vitrified [1 - U - Pu - MA = NVFP][b]

[a] Disposed material form.

[b] MA = minor actinides; TRU = MA + Pu; NVFP = all non-volatile fission products; VLHR = very low heat radio-nuclides; LHR = low heat radio-nuclides; U = uranium. Note that *nsc = 3* and *4* result in two kinds of LHR waste products – with and without Pu; in a later paper (OECD, 2000) Forsberg includes Pu in the LHR mix.

[c] Expressed relative to the indicated scenario (*e.g., nsc = 2 = 1 – U* indicates scenario 1 with uranium removed via UREX process, and the remainder put into vitrified glass, *etc.*)

"Tier-less" Front-end Scenarios for Investigating Repository Impacts

Advanced Accelerator Applicatio

Scenario, *nsc*	Elaborated Comparative Description
1	Base- or Point-of-Departure (POD) case: Direct disposal of SNF fuel assemblies, including most VFPs.
2	Reduce mass and (hopefully) volume, but must deali with full short- and long-term heat loads[(b)].
3	Reduce mass and (hopefully) volume, as well as short-term heat load associated with HHRs, but with full (TRU = Pu + MA) long-term heat load (and proliferation risk).
4	Similar to *nsc = 3*, with some reduction in long-term heat load through the removal of Pu (and reduced long-term proliferation risk).
5	Not unlike *nsc = 2*, but with some reduction in long-term heat load resulting from Pu removal (and reduced long-term proliferation risk).
6	The best it gets; volume and mass reduction along with reductions in both short-term and long-term heat loads.
7	Reduce mass and (hopefully) volume with full short-term heat load, but with significantly reduced long-term heat load.